

# ABSTRACT

Charles University in Prague, Faculty of Pharmacy in Hradec Kralove

Department: Department of Pharmaceutical Chemistry and Drug Control

Candidate: Veronika Krepsova

Supervisor: doc. PharmDr. Petr Zimcik, Ph.D.

Title of Diploma Thesis: Azaphthalocyanines substituted with one aminogroup – distance dependence on photoinduced electron transfer

Azaphthalocyanines (AzaPc), the aza-analogues of phthalocyanines are macrocyclic compounds with large conjugated system and mostly with high quantum yields of singlet oxygen and fluorescence. Intramolecular charge transfer (ICT) was discovered to proceed in AzaPc when alkylamino group is present on AzaPc periphery. ICT is responsible for quenching of excited states causing disappearance of singlet oxygen production and fluorescence emission. The aim of this thesis was to synthesize AzaPcs suitable for studying a similar process called photo-induced electron transfer (PET). In this process donor amino group is not in conjugation with AzaPc macrocycle, electron must “jump” over a distance leading to the quenching of excited states of molecules.

In the first part of my work 5-chloro-6-methylpyrazine-2,3-dicarbonitrile was synthesized using nucleophilic substitution on 5-[2-(diethylamino)ethylsulfanyl]-6-methylpyrazine-2,3-dicarbonitrile (precursor A). The synthesis of unsymmetrical AzaPc was performed *via* statistic condensation of 5,6-bis(*tert*-butylsulfanyl)pyrazine-2,3-dicarbonitrile (precursor B) and the compound A in ratio 3:1. Unsymmetrical congener A<sub>3</sub>B was isolated from the mixture of magnesium congeners by the mean of column chromatography. Magnesium cation was removed from the center of AzaPc giving metal-free derivative and zinc cation was then coordinated into center of AzaPc. Spectral properties of prepared AzaPcs were also studied.

The second part of the thesis concerned with the synthesis of AzaPc where the donor for PET was the aromatic amine in order to obtain different basicity in comparison with compounds investigated in the first part of the thesis. The synthesis was based on the condensation of diaminomaleonitrile with keto acids prepared by cleavage of hydantoin core under basic conditions.